

NASA GRANT NAG-1-244

NUMERICAL SOLUTIONS OF THE COMPLETE
NAVIER-STOKES EQUATIONS

Progress Report No. 16

For the Period July 1, 1988 to December 31, 1989

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(NASA-CR-186102) NUMERICAL SOLUTIONS OF THE
COMPLETE NAVIER-STOKES EQUATIONS Progress
Report No. 16, 1 Jul. 1988 - 31 Dec. 1989
(North Carolina State Univ.) 16 p CSCL 200

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N90-13747

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16p.

During the period an abstract (copy enclosed) was submitted to the 21st AIAA Fluids and Plasmadynamics Conference to be held in June, 1990. It summarizes our efforts in PDF approach to turbulence modelling in the presence of combustion.

A HYBRID REYNOLDS AVERAGED/PDF CLOSURE MODEL
FOR SUPERSONIC TURBULENT COMBUSTION

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Abstract

A hybrid Reynolds averaged/assumed probability density function (PDF) approach has been developed and applied to the study of turbulent combustion in a supersonic mixing layer. This approach is used to address the "laminar-like" treatment of the thermochemical terms that appear in the conservation equations. Calculations were carried out for two experiments involving H₂-Air supersonic turbulent mixing. A SPARK combustion model was employed. In general, the approach shows modest improvement over previous calculations.

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Introduction

The design of an efficient supersonic combustion ramjet (scramjet) requires a fundamental understanding of the interaction between several complex processes that take place within the engine. These processes are dominated by turbulent mixing and its effect upon the chemical reaction. This work is part of a continuous research program designed to better understand processes involving mixing and burning within a supersonic free shear layer. This simulates parallel injection of hydrogen fuel in a scramjet without introducing the complexities arising from the geometry. Earlier attempts used the Reynolds averaged Navier-Stokes equations and an algebraic turbulence model¹. The thermochemical terms that appear in the conservation equations were treated as "laminar-like". That is, the source terms resulting from the chemical nonequilibrium are assumed to depend on mean flow quantities. Because of the exponential dependence of these terms on temperature and because of the short residence time of the fuel-air mixture in scramjet engines, such "laminar-like" assumptions are deemed inappropriate².

The PDF approach for describing turbulent reacting flows³ represents an attractive, yet, untested approach for supersonic combustion. This is because the underlying theory has yet to be developed. Even when the theory becomes available, the computational effort may be rather prohibitive. On the other hand, an assumed PDF approach to handle the thermochemical terms presents a conceptually attractive yet computationally inexpensive approach for dealing with the chemical source terms. The assumed PDF depends on the mean and the variance of the quantity to be averaged. Since Reynolds averaging provides an equation for the mean quantities, the additional cost reduces to solving an extra field equation for each of the additional quantities that appear in the source term.

The source terms depend on the temperature and the concentrations. Rather than assume a joint PDF for the temperature and the concentration, it was assumed that the joint probability function can be written as the product of individual PDF's. For the reactions where the concentration appears as a first power, the above assumption yields mean concentrations. If it is

further assumed that the contribution of recombination reactions are small, then the only PDF that needs to be assumed is that for the temperature.

The results obtained so far, assumed that the PDF of the temperature is Maxwellian, i.e.,

$$P(T) = \frac{1}{(2\pi)^{1/2} \sigma} \exp \left[-\frac{(T - \tilde{T})^2}{\sigma^2} \right] \quad (1)$$

where

$$T = \tilde{T} + T'' \quad (2)$$

and

$$\sigma^2 = \overline{T''^2} = \frac{\overline{\rho T''^2}}{\bar{\rho}} \quad (3)$$

is the variance. Using the results of Jones and Whitelaw⁴, the variance is determined from the Favre -averaged partial differential equation

$$\frac{D}{Dt} (\overline{\rho T''^2}) = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{\sigma_t} \frac{\partial \overline{T''^2}}{\partial x_i} \right) + 2C_1 \frac{\mu_t}{\sigma_t} \left(\frac{\partial \tilde{T}}{\partial x_i} \right)^2 - 2C_2 \frac{V_o}{L} \bar{\rho} \overline{T''^2} \quad (4)$$

where C_1 and C_2 are constants, V_o is the centerline velocity and L is the width of the mixing layer defined in the manner indicated in Ref. 1, μ_t is the turbulent viscosity and σ_t is the turbulent Prandtl number. The calculations presented here used $C_1 = 2.7$ and $C_2 = 0.05$.

The production rate of species s can be represented as

$$\dot{w}_s = \sum_j A_j K_{fj}(T) + \sum_j B_j K_{bj}(T) \quad (5)$$

where A_j and B_j are functions of the concentrations. The average of \dot{w}_s

$$\overline{\dot{w}_s} = \sum_j A_j \int K_{fj}(\tilde{T} + T'') P(T'') dT'' + \sum_j B_j \int K_{bj}(\tilde{T} + T'') P(T'') dT'' \quad (6)$$

The integrals are calculated using a trapezoidal rule.

Results and Discussion

The PDF closure was applied to two reacting H₂-Air coaxial jet flow experiments. The first of which was the experiment conducted by Beach et al. (5), the conditions for which appear in table 1. A schematic of the burner is given in figure 1a.

Figures 2 and 3 show profiles for four species at four axial locations downstream of the jet exit. Figure 2 displays results without the PDF closure and figure 3 shows results with the PDF closure. The results are very similar, but one can notice a slightly greater depletion of O₂ and a slightly higher level of H₂O in the main reaction zone. This is indicative of the greater extent of combustion that seems to be associated with the use of the PDF method. This trend persists at all axial locations, and seems to be in line with what the experiment predicts.

The second reacting jet flow experiment was that performed by Jarrett et al. (6), at the NASA Langley Research Center. The apparatus is shown in figure 1(b). The geometry of this jet causes doubt as to the certainty of the jet exit conditions appearing in table 2, which do not reflect the shock structure emanating from the tip of fuel injector.

Figure 5 shows the temperature profiles at four axial locations. The results obtained with the PDF closure are given by the solid line, and without the PDF closure by the dashed line. With the PDF we see a better prediction of the peak temperature within the mixing layer.

In figure 6 and 7 we have displayed number density profiles of N₂ and O₂, respectively, versus normal distance data at four axial locations. From these plots we see that the extent of mixing is predicted reasonably well. However, the O₂ profiles show that the extent of combustion is overpredicted. It may be recalled that in the present work concentration fluctuations appearing in the expression for the reaction rates were not allowed for. This may explain the cause of our discrepancy. It is possible that, once these fluctuations are properly accounted for, a better prediction of the extent of combustion can also be realized. We chose to consider temperature fluctuations because of the highly non-linear fashion in which they manifest themselves. Allowing for fluctuations in concentrations will most likely be the focus of future work.

Conclusions

Implementation of a new model which better accounts for the effects of turbulence on the chemistry in supersonic reacting flows has been achieved. Here we represented the scalar fluctuations in temperature through the specification of the functional form of the PDF. A more accurate prediction of the peak temperature within the mixing layer of a supersonic reacting stream has been achieved.

Extension of this method to account for fluctuations in species concentrations should yield a more accurate prediction of the extent of combustion. Future work will consider these effects. Investigations are also currently underway to study different forms for the presumed shape of the PDF.

Acknowledgement

This work is supported in part by the following grants: NASA Grant NAG-1-244, the Hypersonic Aerodynamics Research Grant NAGW-1022 funded jointly by NASA, AFOSR and ONR; and the Mars Mission Research Center funded by NASA Grant NAGW-1331. The authors would like to acknowledge many helpful discussions with Dr. Dean R. Eklund of the NASA Langley Research Center.

Table 1

Exit Conditions	Hydrogen Jet	Outer Jet
Mach Number	2.0	1.9
Temperature, K	251	1495
Velocity, m/s	2418	1510
Pressure, MPa	.100	.100
Mass Fraction		
Y_{H_2}	1	0
Y_{O_2}	0	.241
Y_{N_2}	0	.478
Y_{H_2O}	0	.281

Table 2

Exit Conditions	Hydrogen Jet	Outer Jet	Ambient Air
Mach Number	1.	2.02	0.
Temperature, K	545	1250	273.
Velocity, m/s	1772	1441	0
Pressure, Mpa	.112	.096	.101
Mass Fraction			
Y_{H_2}	1	0	0
Y_{O_2}	0	.254	.233
Y_{N_2}	0	.572	.767
Y_{H_2O}	0	.174	0

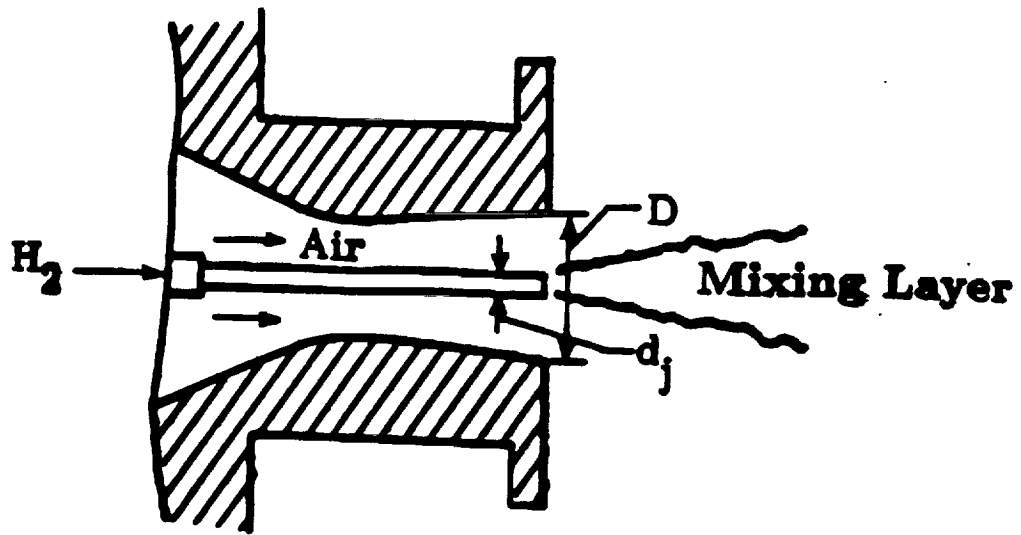


Fig. 1(a). Schematic of Beach coaxial jet flowfield.

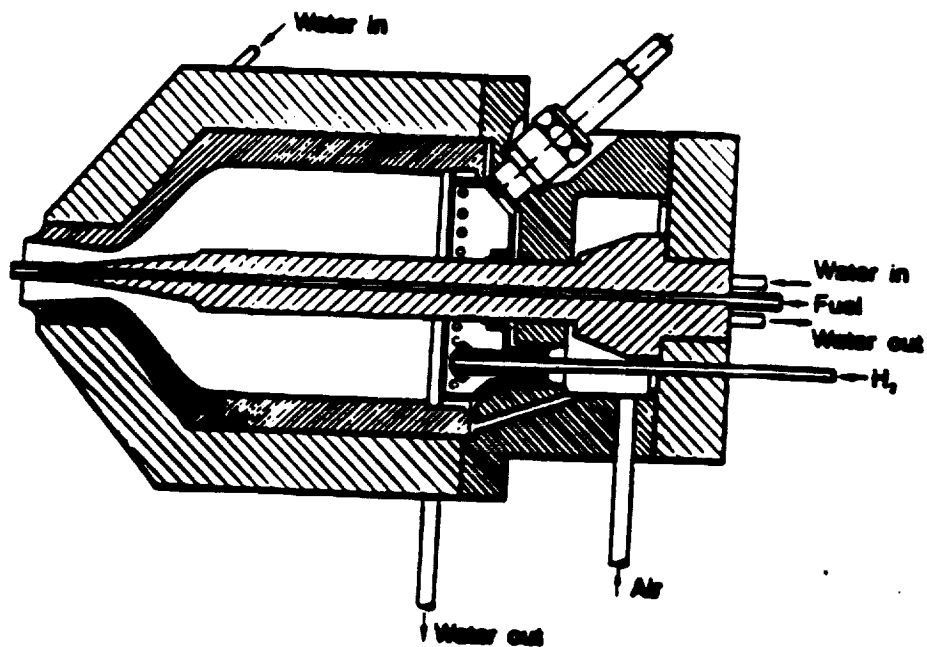


Fig. 1(b). Schematic of the test apparatus for the Jarrett experiment.

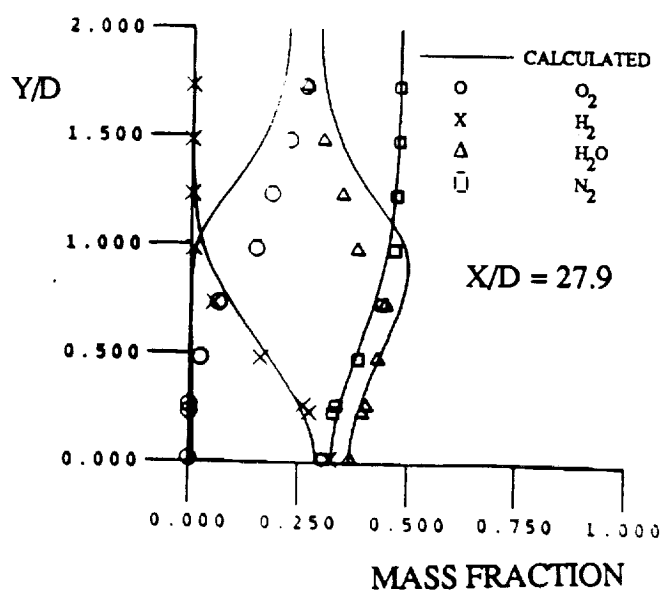
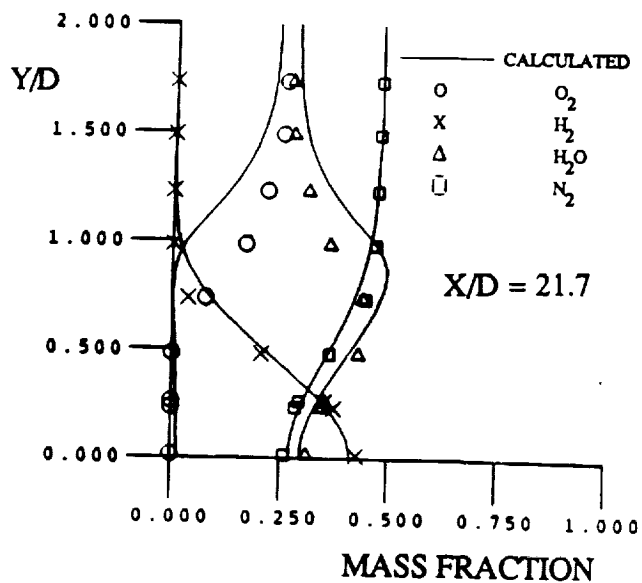
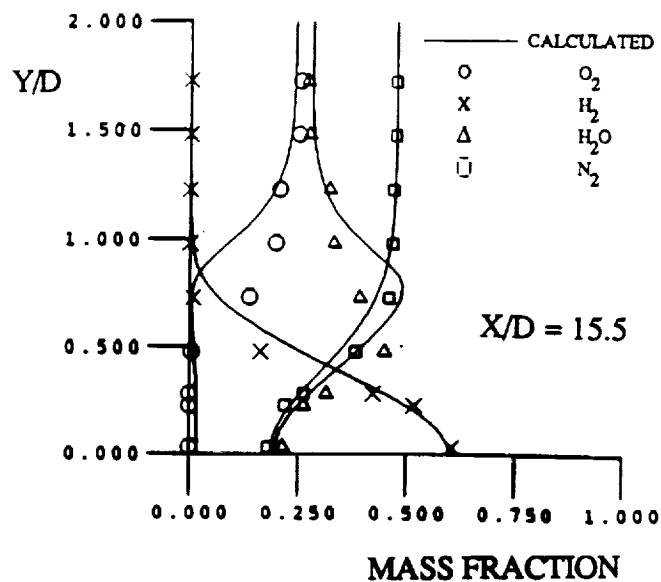
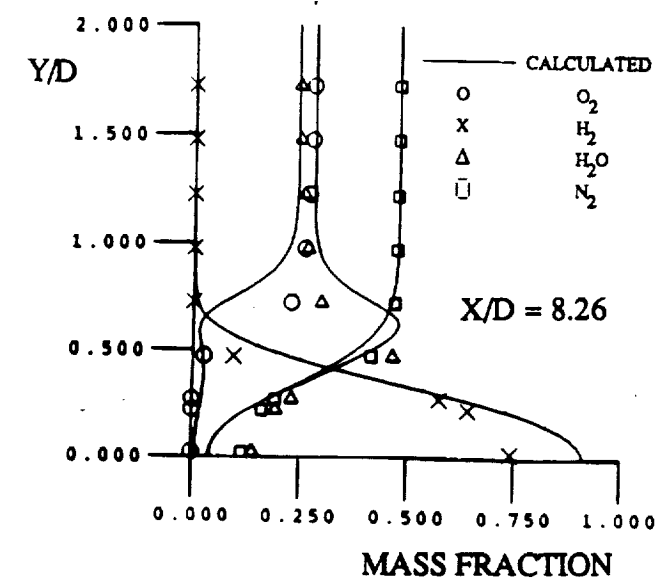


Fig. 2. Mass fraction profiles at four axial locations for the Beach case calculated without the PDF closure.

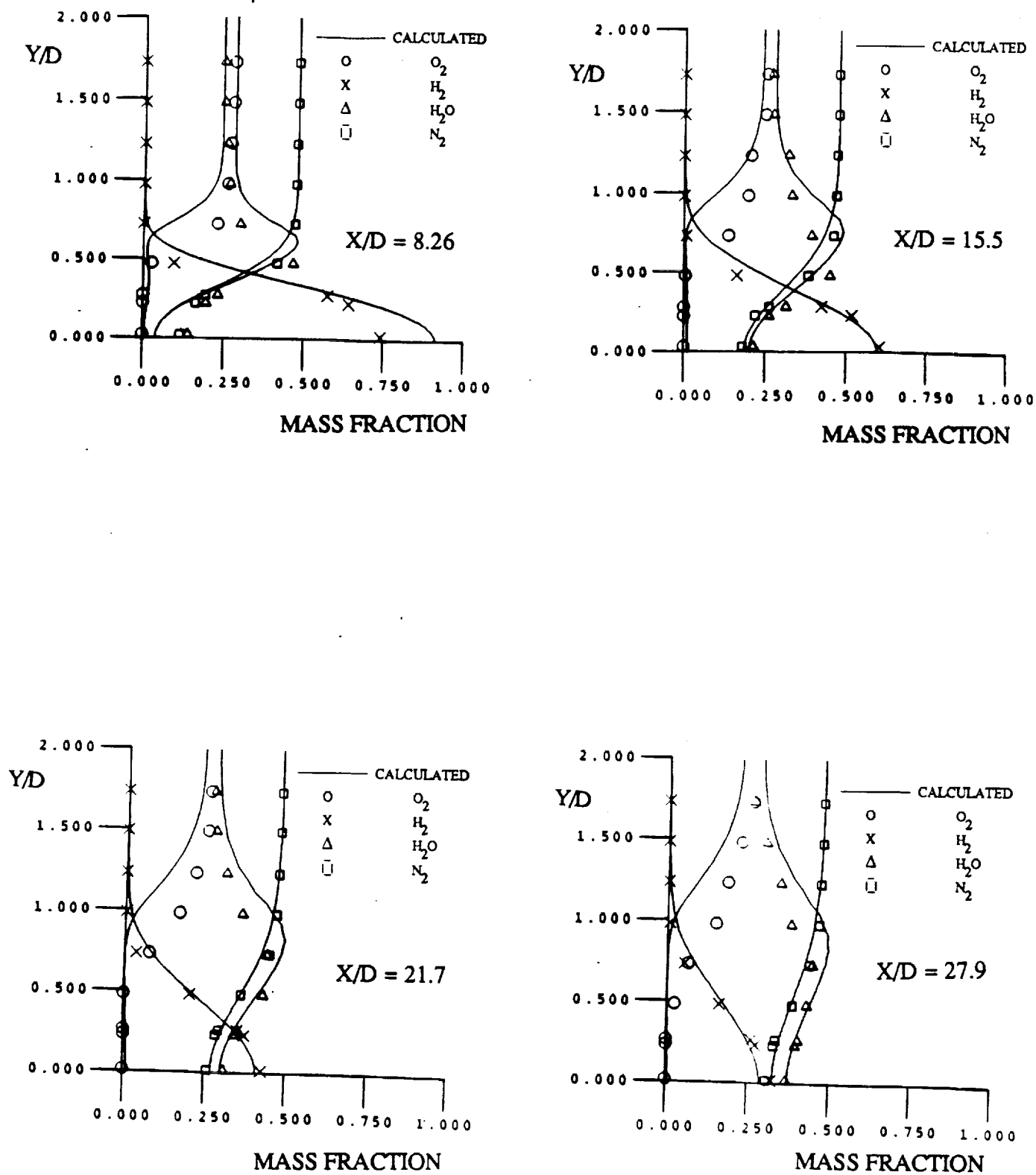


Fig. 3. Mass fraction profiles at four axial locations for the Beach case calculated with the PDF closure.

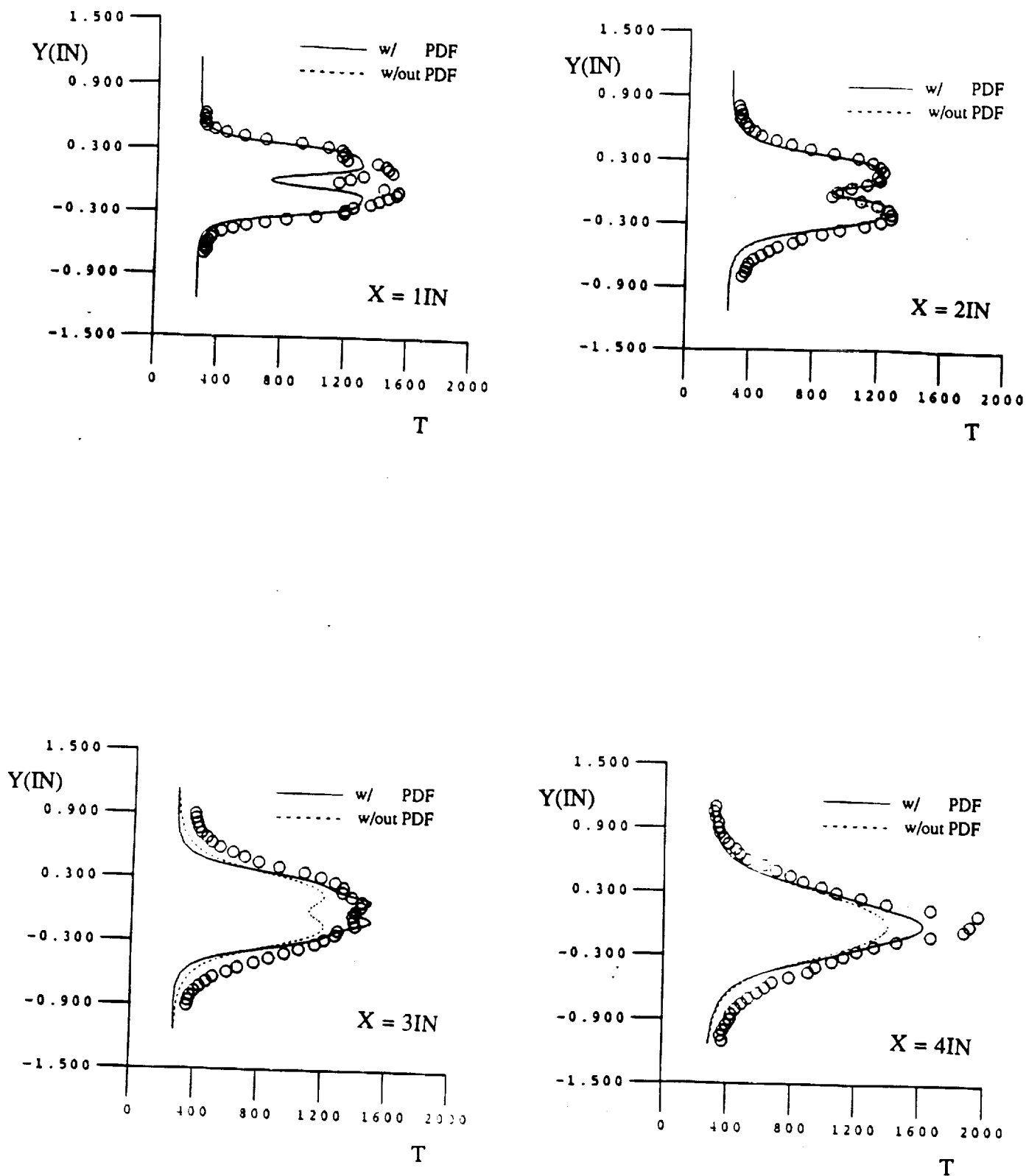


Fig. 4. Temperature (K) profiles at four axial locations for the Jarrett case.

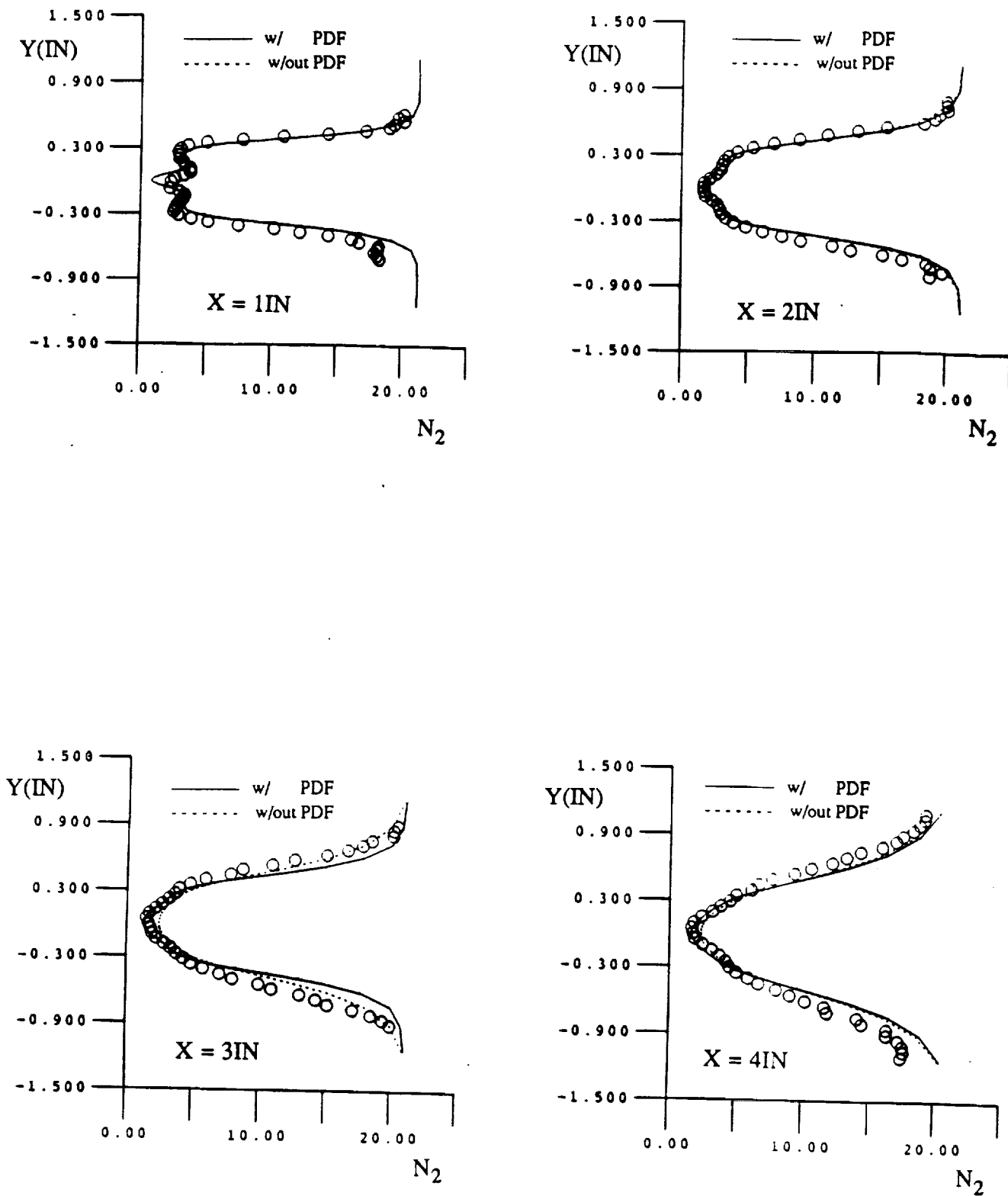


Fig. 5. Nitrogen number density ($\times 10^{-18}$) profiles at four axial locations for the Jarrett case.

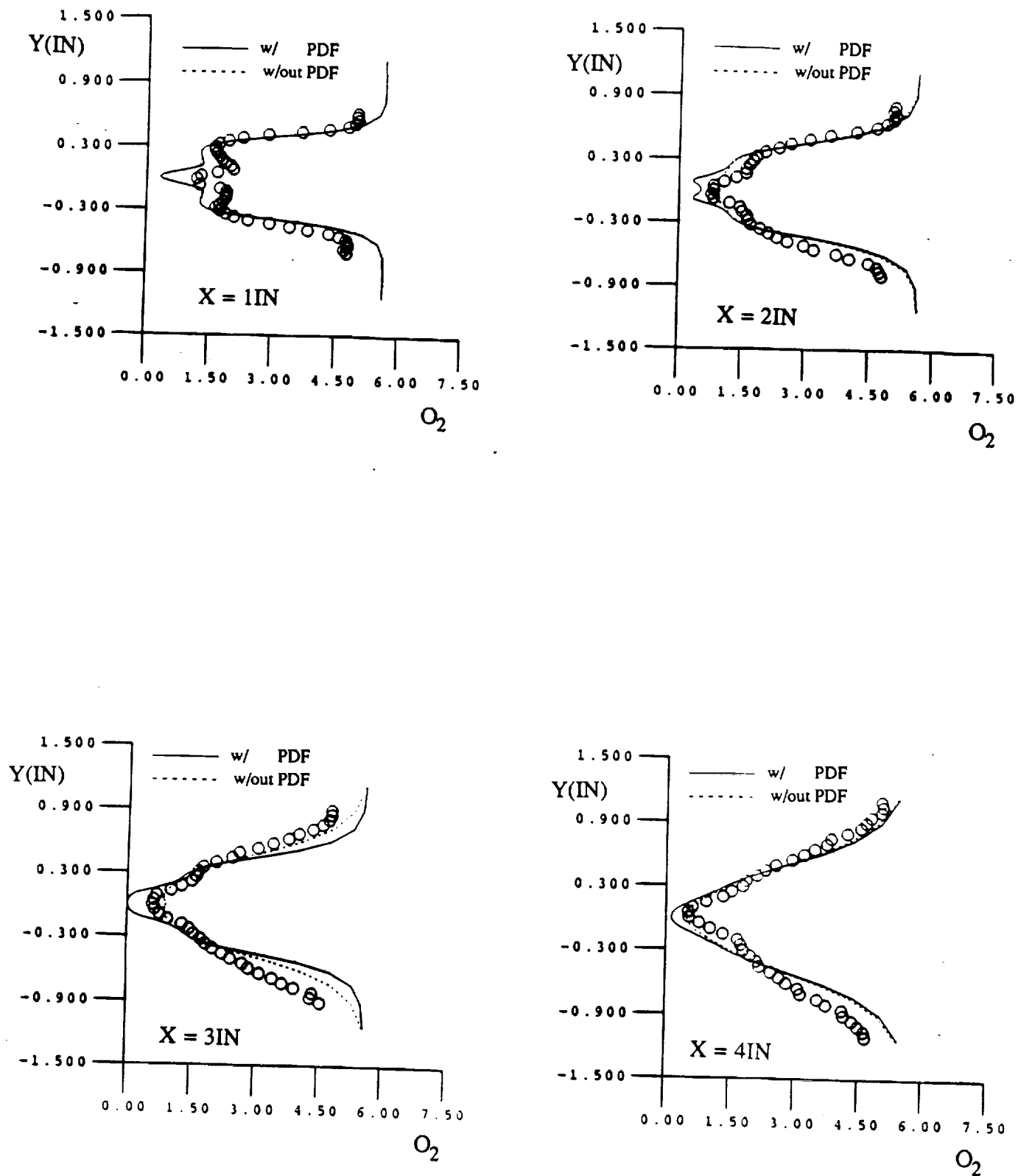


Fig. 6. Oxygen number density ($\times 10^{-18}$) profiles at four axial locations for the Jarrett case.

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